Quantum Fluctuations Affect Critical Properties of Noble Gases *

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Molecular dynamics presents a powerful tool for elucidating the features of mesoscopic systems. The present communication draws attention to the possible importance of quantum fluctuations in such treatments. To illustrate this issue, we focus on the cluster mass distribution for argon atoms in thermal equilibrium.

We have adapted a recently developed quantal Langevin treatment [1,2] to a system of argon atoms in thermal equilibrium. The method was developed in the context of nuclear dynamics and takes approximate account of the energy fluctuations that are necessarily present when wave packets are used to describe the system. The presence of these quantum fluctuations changes the character of the specific heat from classical to quantal and their inclusion by the developed method leads to a significant improvement of the statistical properties in a number of simple test cases that can be subjected to exact analysis [2,3] as well as for finite nuclei [1,2]. When incorporated into microscopic dynamical simulations of nuclear collisions, it leads to a significant improvement of the calculated fragment mass distribution [4].

Our studies suggest that quantum fluctuations inherent in wave packet dynamics may also play a role in atomic physics. As illustrated in fig. 1, the cluster mass distribution for noble gases can be affected significantly. In particular, the critical temperature for argon is reduced by around 20%, which is the value of the factor α entering into the modified Einstein relation. The quantum fluctuations may therefore also affect the formation process and might affect the outcome of dynamical simulations aimed at understanding the observed mass distributions.

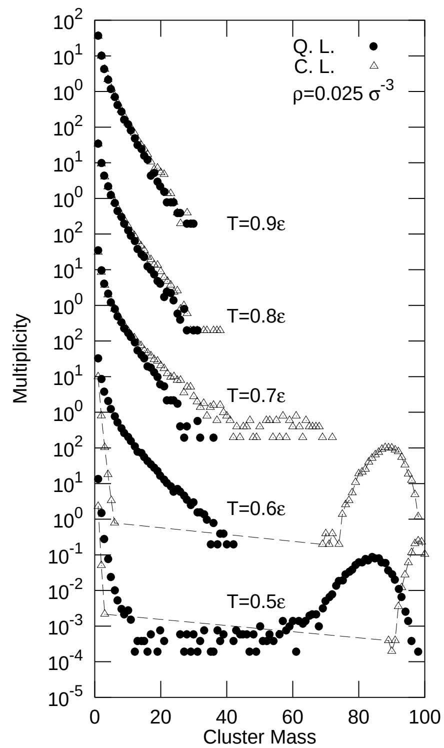

Figure 1: The mass distribution of argon clusters calculated either *with* (solid circle) or *without* (open triangle) the quantum Langevin force emulating the quantum fluctuations inherent in wave-packet dynamics. The argon atoms interact with a Lennard-Jones potential, $V(r) = \epsilon((\sigma/r)^{12} - (\sigma/r)^{6})$; the temperatures are indicated in units of ϵ and the atomic density is $\rho = 0.025\ \sigma^{-3}$.

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[2] A. Ohnishi and J. Randrup, LBL-38596, Ann. Phys. (in press)

[3] A. Ohnishi and J. Randrup, LBNL-39473, Phys. Lett. B (in press)

[4] A. Ohnishi and J. Randrup, LBL-33703, Nucl. Phys. A565 (1993) 474

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